Nonaxial-octupole Y_{32} correlations in $N = 150$ isotones from multidimensional constrained covariant density functional theories

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The non-axial reflection-asymmetric β_{32} shape in some transfermium nuclei with $N = 150$, namely ^{246}Cm, ^{248}Cf, ^{250}Fm, and ^{252}No are investigated with multidimensional constrained covariant density functional theories. By using the density-dependent point coupling covariant density functional theory with the parameter set DD-PC1 in the particle-hole channel, it is found that, for the ground states of ^{248}Cf and ^{250}Fm, the non-axial octupole deformation parameter $\beta_{32} > 0.03$ and the energy gain due to the β_{32} distortion is larger than 300 keV. In ^{246}Cm and ^{252}No, shallow β_{32} minima are found. The occurrence of the non-axial octupole β_{32} correlations is mainly from a pair of neutron orbitals [734]9/2 ($\nu j_{15/2}$) and [622]5/2 ($\nu g_{9/2}$) which are close to the neutron Fermi surface and a pair of proton orbitals [521]3/2 ($\pi f_{7/2}$) and [633]7/2 ($\pi i_{13/2}$) which are close to the proton Fermi surface. The dependence of the non-axial octupole effects on the form of energy density functional and on the parameter set is also studied.

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The majority of observed nuclear shapes is of spheroidal form which is usually described by β_{20}. The existence of the nonaxial-quadrupole (triaxial) deformation β_{22} [1–3] and the axial octupole deformation β_{30} [4] in atomic nuclei have also been confirmed both experimentally and theoretically. However, there is no a priori reason to neglect the nonaxial-octupole deformations, especially the β_{32} deformation [5–7]. The pure β_{32} deformation has a tetrahedral symmetry with a symmetry group T_d^D. The existence of non-trivial irreducible representations of this group makes it possible for a nuclei to have large energy gaps in their single-particle levels, thus increasing it's stability [8]. It has been anticipated that β_{32} deformation occurs in the ground states of some nuclei with special combinations of the neutron and proton numbers [7–9]. Recently, lots of theoretical studies focus on this nuclear shape, either from the T_d^D-symmetric single particle spectra [7, 9–11] or from various nuclear models including the macroscopic-microscopic model [9, 11–13], the Skyrme Hartree-Fock (SHF), SHF+BCS, or Skyrme Hartree-Fock-Bogoliubov models [11–18], and the Reflection Asymmetric Shell Model (RASM) [19, 20]. In particular, Dudek et al. predicted that a negative-parity band in ^{156}Gd is a favorable candidate to manifest tetrahedral symmetry [13] which has stimulated several interesting experimental studies [21, 22].

Nowadays the study of nuclei with $Z \sim 100$ becomes more and more important because it not only reveals the structure of these nuclei themselves but also provides significant information for superheavy nuclei [23–26]. One of the relevant and interesting topics is how to explain the low-lying 2^- states in some $N = 150$ even-even nuclei. In these nuclei, the bandhead energy $E(2^-)$ of the lowest 2^- bands is very low [27]. It is well accepted that the octupole correlation is responsible for it. For example, a quasiparticle phonon model with octupole correlations included was used to explain the excitation energy of the 2^- state of the isotones with $N = 150$ and the octupole correlation is mainly due to the neutron two-quasiparticle configuration $9/2^-[724] \otimes 5/2^+[622]$ and proton two-quasiparticle configurations $9/2^+[633] \otimes 5/2^-[521]$ or $7/2^+[633] \otimes 3/2^-[521]$ [28]. In all these configurations, the third components of the angular momenta of like-quasiparticles K differ by 2, i.e., Y_{32}-correlation should play an important role. In Ref. [20], Chen et al. proposed that the non-axial octupole Y_{32}-correlation results in the experimentally observed low-energy 2^- bands in the $N = 150$ isotones and the RASM calculations reproduces well the experimental observables of these 2^- bands. It was also predicted that the strong nonaxial-octupole effect may persist up to the element 108 [20] and play a crucial role in determining the shell stability in even heavier nuclei [29]. Pronounced shell effects were also found for $N = 16$, 40, and 110 when combining nonaxial octupole deformations [30].

In this Brief Report we present a microscopic and self-consistent study of the Y_{32} effects in the $N = 150$ isotones under the framework of the covariant density functional theory (CDFT) [31–36]. We use the recently developed multi-dimensional constraint (MDC) CDFT [37, 38] in which not only the axial [39, 40] but also the reflection symmetries [41] are broken. For the parametrization of the nuclear shape, the conventional ansatz in mean-field calculations

$$\beta_{\lambda\mu} = \frac{4\pi}{3AR^\lambda}\langle Q_{\lambda\mu}\rangle, \tag{1}$$

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TABLE I. The quadrupole deformation β_{20}, non-axial octupole deformation β_{32}, and hexadecapole deformation β_{40} together with binding energies $E_{\rm cal}$ for the ground states of $N = 150$ nuclei calculated with DD-PC1. $E_{\rm depth}$ denotes the energy difference between the ground state and the point with $\beta_{32} = 0$ in the potential energy curves shown in Fig. 1. $E_{\rm exp}$ denotes experimental binding energies taken from [45]. All energies are in MeV.

Nucleus	β_{20}	β_{32}	β_{40}	$E_{\rm cal}$	$E_{\rm depth}$	$E_{\rm exp}$
^{246}Cm	0.296	0.020	0.126	−1847.932	0.034	−1847.819
^{248}Cf	0.299	0.037	0.111	−1857.853	0.351	−1857.776
^{250}Fm	0.293	0.034	0.097	−1865.843	0.328	−1865.520
^{252}No	0.293	0.025	0.083	−1872.133	0.104	−1871.305

is adopted, where $Q_{\lambda\mu} = r^\lambda Y_{\lambda\mu}$ is the mass multipole operator. The nuclear shape is assumed to be invariant under the reversion of x and y axes in MDC-CDFT, i.e., the intrinsic symmetry group is V_4 and all shape degrees of freedom $\beta_{\lambda\mu}$ deformations with even μ are allowed. The CDFT functional can be one of the following four forms: the meson exchange or point-coupling nucleon interactions combined with the non-linear or density-dependent couplings [37, 38]. In the present work, the pairing effect is taken into account by using the BCS approximation with a separable pairing force [42–44].

First we study the ground states of nuclei ^{246}Cm, ^{248}Cf, ^{250}Fm, and ^{252}No by using the density-dependent point coupling covariant density functional theory with the parameter set DD-PC1 in the particle-hole channel [46]. The quadrupole deformations β_{20}, non-axial octupole deformation β_{32}, and hexadecapole deformations β_{40} together with binding energies $E_{\rm cal}$ are listed in Table I. The non-axial quadrupole and axial octupole deformation parameters are all zero for these nuclei. As is seen in Table I, the calculated binding energies agree very well with the data. All of these four nuclei are well deformed with the quadrupole deformation parameter $\beta_{20} \approx 0.3$ and the hexadecapole deformations $\beta_{40} \approx 0.1$. Superposed with large quadrupole and hexadecapole deformations, finite values are obtained for the non-axial octupole deformation β_{32} for these $N = 150$ isotones.

In order to see more clearly the development of non-axial octupole β_{32} deformation along the $N = 150$ isotonic chain, we preform one-dimensional constrained calculations and obtain potential energy curves, i.e., the total binding energy as a function of β_{32}. At each point of a potential energy curve, the energy is minimized automatically with respect to other shape degrees of freedom such as β_{20}, β_{22}, β_{30}, and β_{40}, etc. In Fig. 1, we show potential energy curves for these $N = 150$ isotones. For ^{246}Cm, the ground state deformation $\beta_{32} = 0.020$ (see Fig. 1 as well as Table I). The potential energy curve is rather flat around the minimum. We denote the energy difference between the ground state and the point with $\beta_{32} = 0$ by $E_{\rm depth}$ which measures the energy gain with respect to the β_{32} distortion. For ^{246}Cm, $E_{\rm depth}$ is

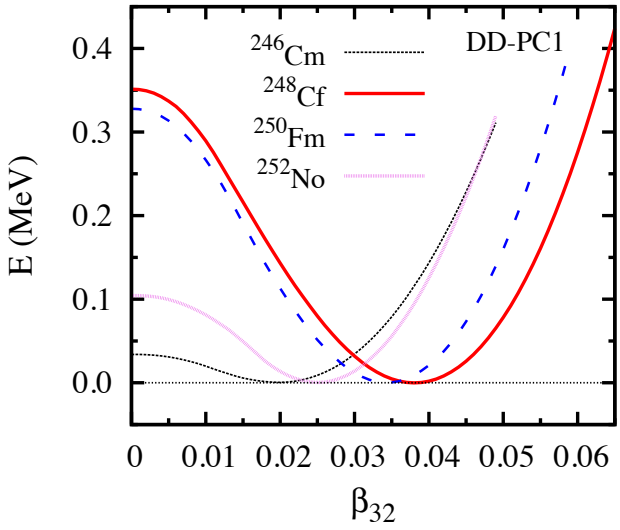

FIG. 1. (Color online) The binding energy E (relative to the ground state) for $N = 150$ isotones ^{246}Cm (dashed line), ^{248}Cf (solid line), ^{250}Fm (long-dashed line), and ^{252}No (dotted line) as a function of the non-axial octupole deformation parameter β_{32}.

only 34 keV. For ^{248}Cf, ^{250}Fm and ^{252}No, the minima locate at $\beta_{32} = 0.037$, 0.034, and 0.025, respectively. The corresponding energy gain $E_{\rm depth} = 0.351$, 0.328, and 0.104 MeV. It may be hard to conclude that these nuclei have static non-axial octupole deformations from these results because the potential energy curve is flat around the minimum and $E_{\rm depth}$ is small. However, the present calculations at least indicate a strong Y_{32}-correlation in these nuclei. Both the non-axial octupole parameter β_{32} and the energy gain $E_{\rm depth}$ reach maximal values at ^{248}Cf in the four nuclei along the $N = 150$ isotonic chain. This is consistent with the analysis given in Refs. [20, 28] and the experimental observation that in ^{248}Cf, the 2^- state is the lowest among these nuclei.

The triaxial octupole Y_{32} effects stem from the coupling between pairs of single-particle orbits with $\Delta j = \Delta l = 3$ and $\Delta K = 2$ where j and l are the total and orbit angular momentum of single particles respectively and K the projection of j on the z axis. If the Fermi surface of a nucleus lies close to a pair of such orbitals and these two orbitals are nearly degenerate, a strong non-axial octupole β_{32} effect is expected.

In Fig. 2, we show the proton and neutron single-particle levels near the Fermi surface for ^{248}Cf as functions of quadrupole deformation β_{20} on the left side and of β_{32} with β_{20} fixed at 0.3 on the right side. In Fig. 2(a), one finds a strong spherical shell closure at $Z = 92$. As discussed in Ref. [47], this shell closure is a spurious one and it is commonly predicted in relativistic mean field calculations. The spherical proton orbitals $\pi 2f_{7/2}$ and $\pi 1i_{13/2}$ are very close to each other and this near degeneracy results in octupole correlations. The two proton levels, [521]3/2 originating from $2f_{7/2}$ and [633]7/2 originating from $1i_{13/2}$, satisfying the $\Delta j = \Delta l = 3$ and

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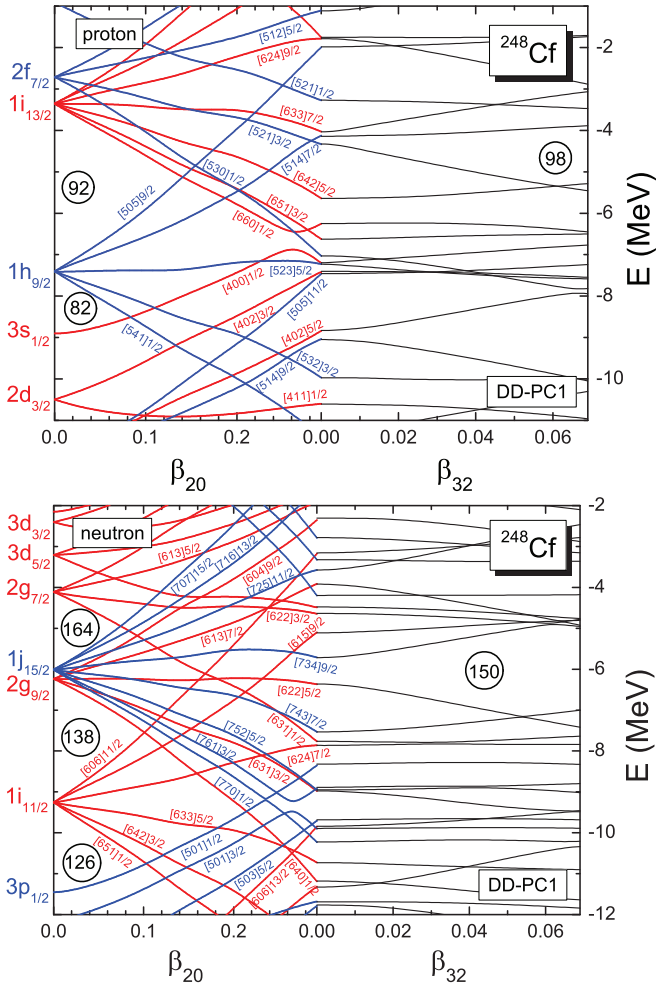

FIG. 2. (Color online) The single-particle levels near the Fermi surface for (a) protons and (b) neutrons of ^{248}Cf as functions of quadrupole deformation β_{20} (left side) and of β_{32} with β_{20} fixed at 0.3 (right side).

$\Delta K = 2$ condition, are very close to each other when β_{20} varies from 0 to 0.3. Therefore the non-axial octupole Y_{32} develops and with β_{32} increasing from zero, an energy gap appears at $Z = 98$. The appearance of the spurious shell closure at $Z = 92$ is mainly due to the lowering of $\pi 1h_{9/2}$ orbital which also results in that the proton [514]7/2 level lies in between [521]3/2 and [633]7/2, thus making the gap at $Z = 98$ smaller and weakening the Y_{32} correlation. Similarly, the spherical neutron orbitals $\nu 2g_{9/2}$ and $\nu 1j_{15/2}$ are very close to each other. The two neutron levels, [734]9/2 originating from $1j_{15/2}$ and [622]5/2 originating from $2g_{9/2}$, are also close to each other and they just lie above and below the Fermi surface. This leads to the development of a gap at $N = 150$ with β_{32} increasing. Therefore it is clear that the Y_{32} correlation in $N = 150$ isotones is from both protons and neutrons and for ^{248}Cf the correlation is the most pronounced. The gap around $N = 150$ is larger than that around $Z = 98$, which may indicate that the non-axial octupole effect originating from neutrons is larger than that from protons. If there is not a spurious shell gap at $Z = 92$, one can expect more pronounced non-axial octupole correlations from protons.

TABLE II. The quadrupole deformation β_{20}, octupole deformation β_{32}, hexadecapole deformation β_{40} together with binding energies E for the ground states of $N = 150$ nuclei calculated with parameter sets PC-PK1, DD-ME1, DD-ME2 and DD-PC1. $E_{\rm depth}$ denotes the energy difference between the ground states and the point constrained β_{32} to zero. All energies are in MeV.

Nucleus	Parameters	β_{20}	β_{32}	β_{40}	E	$E_{\rm depth}$
^{246}Cm	PC-PK1	0.304	0.0	0.129	−1846.273	—
	DD-ME1	0.297	0.0	0.126	−1847.205	—
	DD-ME2	0.296	0.0	0.125	−1846.662	—
	DD-PC1	0.296	0.020	0.126	−1847.932	0.034
^{248}Cf	PC-PK1	0.306	0.031	0.113	−1857.327	0.139
	DD-ME1	0.299	0.035	0.107	−1857.718	0.278
	DD-ME2	0.300	0.039	0.105	−1857.088	0.474
	DD-PC1	0.299	0.037	0.111	−1857.853	0.351
^{250}Fm	PC-PK1	0.302	0.029	0.098	−1865.301	0.128
	DD-ME1	0.293	0.033	0.093	−1866.425	0.305
	DD-ME2	0.292	0.034	0.091	−1865.505	0.416
	DD-PC1	0.293	0.034	0.097	−1865.843	0.328
^{252}No	PC-PK1	0.300	0.013	0.085	−1870.414	0.001
	DD-ME1	0.293	0.023	0.080	−1873.412	0.089
	DD-ME2	0.292	0.024	0.078	−1872.235	0.125
	DD-PC1	0.293	0.025	0.083	−1872.133	0.104

In order to examine the dependence of our results on the functional form and on the effective interaction, we also studied ^{246}Cm, ^{248}Cf, ^{250}Fm, and ^{252}No with other covariant density functionals and several other typical parameter sets, including PC-PK1 [48], DD-ME1 [49], and DD-ME2 [50]. The results are listed in Table II.

Roughly speaking, the results are similar with different parameter sets: β_{22} and β_{30} vanish in all cases and for a specific nucleus, the calculated β_{20} and β_{40} and the binding energy E with different parametrizations agree with each other. For ^{246}Cm, three parameter sets PC-PK1, DD-ME1, and DD-ME2 predict zero β_{32}. With DD-PC1, as discussed before, a rather shallow potential energy curve with a minimum at $\beta_{32} = 0.020$ is obtained. This indicates that the octupole correlation in ^{246}Cm is very weak. Both from the value of β_{32} and from the energy gain $E_{\rm depth}$ due to the β_{32} distortion, it is found that the density-dependent functionals gives stronger Y_{32} effects than the functional with nonlinear self coupling does. Among the density-dependent functionals, the meson exchange nucleon interaction with the parameter set DD-ME2 gives the largest energy gain $E_{\rm depth}$ for ^{248}Cf, ^{250}Fm, and ^{252}No. The evolution of the non-axial octupole β_{32} effects along the $N = 150$ isotonic chain is almost independent of the form of energy density functional and the parameter set: The Y_{32} effects is the strongest in ^{248}Cf except for that DD-ME1 gives a smaller energy gain for ^{248}Cf than for ^{250}Fm.

In summary, we studied the non-axial octupole Y_{32} effects in $N = 150$ isotones ^{246}Cm, ^{248}Cf, ^{250}Fm, and ^{252}No by using multi-dimensional constraint covariant density functional theories. Due to the interaction between a pair of neutron orbitals, [734]9/2 originating from $\nu j_{15/2}$ and [622]5/2 originating from $\nu g_{9/2}$, and that of a pair of proton orbitals, [521]3/2 originating from $\pi f_{7/2}$ and [633]7/2 originating from $\pi i_{13/2}$, rather strong non-axial octupole Y_{32} effects have been found for ^{248}Cf and ^{250}Fm which are both well deformed with large axial-quadrupole deformations, $\beta_{20} \approx 0.3$. For ^{246}Cm and ^{252}No, a shallow minima develops along the β_{32} deformation degree of freedom. The evolution of the non-axial octupole β_{32} effect along the $N = 150$ isotonic chain is not very sensitive to the form of the energy density functional and the parameter set we used. Finally we note that a nucleus with a very flat potential energy curve $E \sim \beta_{32}$ may not have a static non-axial octupole β_{32} deformation. The ground state wave function should be a strongly correlated superposition of different shapes with similar energies. This suggests that further investigations of these nuclei should include beyond mean field effects by using, for example, the generator coordinate method [16, 51].

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